Supplementary Material

Perfluoropropionic acid ($CF_3CF_2C(O)OH$): Three conformations and dimer formation

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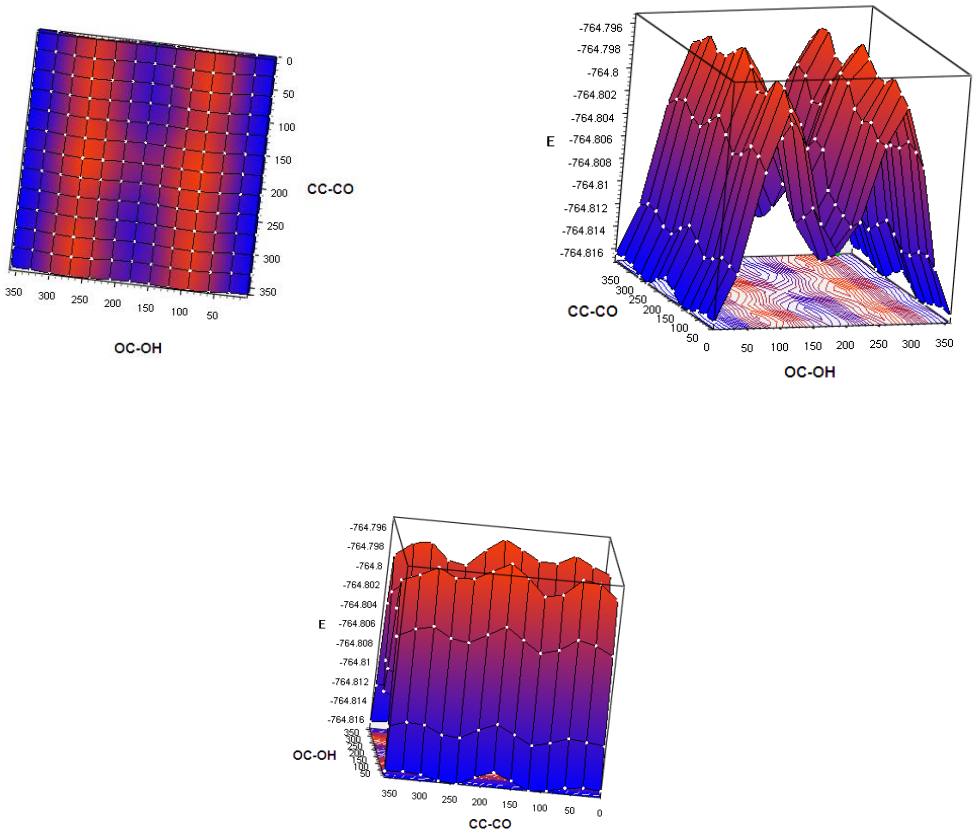

Figure S1. Potential energy surface of $CF_3CF_2C(O)OH$ as a function of the dihedral angles φ(O−C−O−H) and φ(C−C−C=O), displayed from different perspectives.

Table S1. Comparison between experimental and computed IR vibrational modes for $CF_3CF_2C(O)OH$ and their proposed assignment.

Experimental				MP2/6-311+G(D)[a]								Proposed assignament
Gas Phase		Matrix $CF_3CF_2C(O)OH$:Ar (1:500)		*gauche-syn*		*gauche-anti*		*syn-syn*		Dimer		
ν / cm^{-1}	Int	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	
3576	0.204	3574				3586	<1					ν(O–H)
		3547	0.113	3556	23			3556	4			
3107	0.087	3228	0.083							3276	100	
1821	0.284	1834				1767	<1					ν(C=O)
		1813	0.187	1751	66							
		1805	0.076					1745	11			
1779	0.355	1775	0.393							1732	32	
1446	0.056	1457	0.051							1411	5	ν(C2–C3)
		1447	0.049									
1395	0.055	1403	0.028					1359	4			
		1393	0.044	1351	13							
		1378	0.040					1338	2			ν(C3–4)
		1372	0.043									
		1366	0.047			1326	<1					ν(C2–3)
1339	0.192	1335	0.307	1307	23							ν(C3–4)
										1306	11	
						1302	<1					
1279	0.091	1290	0.197							1245	10	δ_{sciss}(COH)
1235	1.000	1240	0.372			1201	<1					$\nu_{as}(CF_3)$
				1197	20							δ_{sciss}(COH)

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Gas Phase		Matrix $CF_3CF_2C(O)OH$:Ar (1:500)		*gauche-syn*		*gauche-anti*		*syn-syn*		Dimer		
ν / cm^{-1}	Int	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	
								1192	15			$\nu_{as}(CF_3)$
		1236	0.752							1189	16	
		1224	1.000			1188	<1					$\delta_{sciss}(COH)$
				1183	85							$\nu_{as}(CF_3)$
										1182	40	
								1181	5			
				1173	38							
1205	0.205	1208	0.323			1168	<1					
								1167	10			$\delta_{sciss}(COH)$
		1203	0.263							1162	4	$\nu_{as}(CF_2)$
1173	0.391	1193	0.15			1153	<1					
		1174	0.634	1144	44							
										1136	26	$\nu_{s}(CF_2)$
								1121	7			$\nu_{as}(CF_2)$
1134	0.217	1142	0.109					1115	4			$\nu_{s}(CF_2)$
		1136	0.175	1108	61							$\nu_{s}(CF_2)$
		1122	0.133			1086	<1					$\nu_{as}(CF_2)$
1034	0.397	1040	0.363							1002	17	$\nu_{s}(CF_3)$
		1035	0.604	996	35							
		1019	0.11					994	13			
						989	<1					
900	0.037	922	0.186							827	12	$\delta_{wagg}(COH)$

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Gas Phase		Matrix $CF_3CF_2C(O)OH$:Ar (1:500)		*gauche-syn*		*gauche-anti*		*syn-syn*		Dimer		
ν / cm^{-1}	Int	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	
								754	1			
775	0.044	791	0.116							752	1	δ(OCO)
		771	0.112	745	6							δ_{wagg}(COH)
						739	<1					$\delta_s(CF_3)$
		763	0.119	735	<1			737	<1			
						730	<1					δ_{wagg}(COH)
										728	2	δ_{twist}(COH)
714	0.094	717	0.167							675	5	δ_{sicss}(OCO)
		712	0.157									
		701	0.086									
676	0.163	682	0.079			667	<1					
		673	0.130					653	5			
				651	26							
621	0.071							631	<1			$\delta_{sicss}(CF_2)$
		622	0.102	610	24	586	<1					δ(COH)
		616	0.141							590	<1	
580	0.034							580	2			
				584	1							$\delta_{sicss}(CF_3)$
		579	0.064			562	<1					δ(COH)
										554	1	δ_{twist}(COH)
								547	3			
543	0.059	542	0.082	527	4							

Experimental				MP2/6-311+G(D)[a]								Proposed assignament
Gas Phase		Matrix $CF_3CF_2C(O)OH$:Ar (1:500)		*gauche-syn*		*gauche-anti*		*syn-syn*		Dimer		
ν / cm^{-1}	Int	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	
						519	<1			519	1	$\delta_{sicss}(CF_3)$
		525	0.031	518	3							$\delta_{sicss}(CF_2)$
						494	<1	514	<1	504	1	$\delta_{sicss}(CF_3)$
						488	<1					$\delta_{wagg}(COH)$
				482	2							$\delta_{sicss}(CF_3)$
								402	<1			$\delta_{twist}(CF_3)$
								400	<1			$\delta_{sicss}(CF_3)$
										380	1	$\delta_{twist}(CF_3)$
						371	<1					$\delta_{sicss}(CF_2)$
										370	<1	$\delta_{sicss}(CF_2)$
				366	<1							δ(OCO)
				362	<1							$\delta_{twist}(CF_3)$
						360	<1					δ(OCO)
				344	<1	343	<1	347	<1	345	<1	$\delta_{wagg}(CF_3)$
								325	<1			δ(OCO)
										287	1	$\delta_{twist}(CF_2)$
				278	<1	279	<1	270	<1	277	1	$\delta_{wagg}(CF_2)$
				243	<1	256	<1	243	<1			$\delta_{twist}(CF_2)$
				208	<1	206	<1	207	<1	209	<1	$\delta_{twist}(CF_3)$
				141	<1	138	<1	149	<1	143	<1	$\delta_{sciss}(CCC)$
										97	<1	δ(OCO)
										70	<1	τ(H···O)

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Gas Phase		Matrix $CF_3CF_2C(O)OH$:Ar (1:500)		*gauche-syn*		*gauche-anti*		*syn-syn*		Dimer		
ν / cm^{-1}	Int	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	ν / cm^{-1}	Int.	
				69	<1	72	<1	91	<1	43	<1	τ(C3−C4)
										13	<1	δ_{sciss}(OH···O)
				24	<1	38	<1	28	<1	9	<1	τ(C2−C3)

[a]Corrected with a scaling factor of 0.95.

Table S2. Crystallographic information for $CF_3CF_2C(O)OH$.

	$C_3HF_5O_2$
Formula weight	164.032
Temperature/K	156.0(1)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.9411(16)
b/Å	5.0964(6)
c/Å	9.7342(13)
β/°	107.431(14)
Volume/Å^3	517.85(13)
Z	4
ϱ_{calc}g/cm^3	2.104
μ/mm^{-1}	0.276
F(000)	320.5
Crystal size/mm^3	0.3 × 0.13 × 0.13
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	7.8 to 50.08
Index ranges	−12 ≤ h ≤ 13, -5 ≤ k ≤ 6, -10 ≤ l ≤ 11
Reflections collected	2583
Independent reflections	902 [R_{int} = 0.0311, R_{sigma} = 0.0368]
Data/restraints/parameters	902/0/95
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0306, wR_2 = 0.0605
Final R indexes [all data]	R_1 = 0.0401, wR_2 = 0.0654
Largest diff. peak/hole / e Å^{-3}	0.33/−0.21

CCDC 1471202 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.